Theor Chim Acta (1992) 83: 3

Theoretica Chimica Acta

Foreword: the width of theoretical chemistry

Theoretical Chemistry, which is the title theme of this Journal, in principle should comprise all theoretical, i.e. scientific concepts being relevant to the liberal art of chemistry. However, during the past two centuries the meaning of the term "theoretical chemistry" has shifted from what is now called "general chemistry" via "physical chemistry" to the subfields of thermodynamics and microscopic theories of matter, and finally to "quantum chemistry" in particular, which itself has become a broad field in the course of development and specialization of the sciences.

So, quantum chemistry comprises many aspects beginning with the basic foundations of quantum theory; the development of mathematical and computational techniques for the solution of molecular quantum-mechanical problems; their application to specific problems of structure, transitions, and reactivity of individual systems; the derivation of approximation schemes with more-or-less empirical loans; the formulation of simple classifying rules of practical use for the experimentalist; and finally bridges between intuitive chemical thinking and rigorous theoretical results. These latter aspects are of profound importance to both the advance of science, the understanding of nature through science, and to the continuity of scientific tradition by teaching.

Among the prominent scientists of the second half of this century, who have contributed in depth and in this width to quantum chemistry, who have advanced the feasibility of reliable theoretical approaches through the invention of mathematical techniques as well as through the development of computationally practical methods, who have solved general and specific problems of molecular structure, spectra and reaction surfaces, who have created definitive interpretative concepts of chemical bonding and molecular wavefunctions, Professor Klaus Ruedenberg would be mentioned as an outstanding representative.

On the occasion of Professor Ruedenberg's seventieth birthday it was decided to organize an International Symposium, and also to edit a special volume of Theoretica Chimica Acta, a favorite foster-child of Prof. Ruedenberg. Both the honorary conference and the special issues of Theoretica Chimica Acta should reflect the width of Prof. Ruedenberg's contributions to the different branches of quantum chemistry being based on rigorous approaches. All participants of the Symposium on *Ab initio* Methods in Quantum Chemistry held at Ames, Iowa, May 9–11, 1991, are grateful to the basic and definite contributions which Prof. Ruedenberg has made to our science, and we also express our thanks to the conference organizers S. T. Elbert and A. Komornicki. The photo of Prof. Ruedenberg on the facing page formed the center of the symposium poster.

The present guest editor, who was attached with TCA during his Ph.D. work in Frankfurt-on-Main when the Journal had just been founded by the late Professor Hartmann, is grateful to Springer-Verlag for the honorable opportunity to take care of a series of issues of TCA with papers from different branches of Quantum Chemistry, all dedicated to Prof. Klaus Ruedenberg, the second and present Editor in Chief.

W. H. Eugen Schwarz, Siegen